

ON G/A – SZEGED INDEX OF STANDARD GRAPHS

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ABSTRACT

A modern graph invariant is Szeged Index and it has considerable applications in molecular chemistry. A recently introduced graph invariant is G/A – Szeged Index and it has a numerable applications in chemistry. In this paper, the G/A – Szeged indices of standard graphs are calculated. A modified G/A – Szeged Index of a graph is also introduced in which all the vertices of the graph are taken into consideration, thereby the variations in these indices of standard graphs are identified.

Keywords: Szeged Index, G/A – Szeged Index, modified G/A – Szeged Index.

1. INTRODUCTION

The useful concepts related to a molecular graph associated with alkanes are mainly Wiener index (See[5]) and Szeged index (see[3]). A recently introduced concept (see [2]) is GA₂ Index and we coined it as G/A– Szeged Index (Geometric mean by Arithmetic mean – Szeged Index). As usual, no standard formula is available to find out this index as well, for any connected graph. In §2, we calculate the G/A – Szeged indices of standard graphs and in §3, we introduce modified G/A – Szeged index and observe the variation of these indices for the standard graphs.

Throughout this paper, we consider only non-empty, simple, finite and connected graph to avoid trivialities.

For the standard notation and results we refer Bondy & Murthy [1].

For ready reference, we give the following:

Definition 1.1 [3]: G is a (non-empty, simple, finite and connected) graph with vertex set V(G) and edge set E(G). Then the Szeged index of G, denoted by Sz(G), is defined to be $\sum_{e \in E(G)} n_1(e).n_2(e)$, where $e = uv$, $N_1(e|G) = \{w \in V(G) : d(w, u) < d(w, v)\}$, $N_2(e|G) = \{w \in V(G) : d(w, v) < d(w, u)\}$ and $n_1(e|G) = |N_1(e|G)|$, $n_2(e|G) = |N_2(e|G)|$. ('d' denotes the distance function and '|'|, the cardinality function).

When there is only one graph G, under consideration, we write 'e' only instead of 'e|G'.

Observations 1.2 [4]:

- a) For the graph K_n (n ≥ 2), Sz(K_n) = n(n-1)/2.
- b) For the complete graph K_{m, n} (m, n ≥ 1), Sz(K_{m, n}) = (mn)².
- c) For the cycle C_k (k ≥ 3), Sz(C_k) = k $\left[\frac{k}{2} \right]^2$ ([] denotes integral part).
- d) For the path P_n (n ≥ 2), Sz(P_n) = n (n² - 1)/6.
- e) For the wheel (K₁ v C_n) (n ≥ 3), Sz(K₁ v C_n) = n $\left\{ (n-2) + \left[\frac{n}{2} \right]^2 \right\}$.

2. G/A – SZEGED INDEX OF STANDARD GRAPHS

For convenience, we recollect the following:

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Definition 2.1 [2]: G is a graph (i.e non- empty, simple, finite and connected graph). Let 'e' be any edge of G. Then the

G/A – Szeged index of G is defined to be $\sum_{e \in E(G)} \frac{\sqrt{n_1(e)n_2(e)}}{[n_1(e) + n_2(e)] / 2}$.

Theorem 2.2: For the complete graph K_n ($n \geq 2$), $G/A - Sz(K_n) = n(n-1)/2$.

Proof: For any $e \in E(K_n)$, by Th.2.3 in [4], $n_1(e) = n_2(e) = 1$.

$$\begin{aligned} \text{So } G/A - Sz(K_n) &= \sum_{e \in E(K_n)} 2 \frac{\sqrt{(1)(1)}}{(1+1)} \\ &= |E(K_n)| \\ &= \frac{n(n-1)}{2}. \end{aligned}$$

Theorem 2.3: For the complete bipartite graph $K_{m, n}$ ($m, n \geq 1$),

$$G/A - Sz(K_{m, n}) = \frac{2(mn)^{3/2}}{m+n}.$$

Proof: For $e \in E(K_{m,n})$, by Th.(2.5) in [4], $n_1(e) = n$ and $n_2(e) = m$, further $|E(K_{m,n})| = mn$.

$$\begin{aligned} \text{So } G/A - Sz(K_{m,n}) &= \sum_{e \in E(K_{m,n})} 2 \frac{\sqrt{(n)(m)}}{(n+m)} \\ &= 2 \frac{\sqrt{(m)(n)}}{(m+n)} |E(K_{m,n})| \\ &= \frac{2(mn)^{3/2}}{m+n}. \end{aligned}$$

Theorem 2.4: For the cycle C_k ($k \geq 3$), $G/A - Sz(C_k) = k$.

Proof: Clearly $|E(C_k)| = k$.

We divide this into two cases.

Case (i): k is even and say $k = 2n$ ($n \geq 2$).

For any $e \in E(C_{2n})$, by Th. (2.6) in [4], $n_1(e) = n_2(e) = n$.

$$\begin{aligned} \text{So } G/A - Sz(C_{2n}) &= \sum_{e \in E(C_{2n})} \frac{2\sqrt{(n)(n)}}{n+n} \\ &= |E(C_{2n})| = 2n. \end{aligned}$$

Case (ii): k is odd and any say $k = 2n-1$ ($n \geq 2$). For any $e \in E(C_{2n-1})$, by Th. 2.6 in [4], $n_1(e) = n_2(e) = n-1$.

$$\begin{aligned} \text{So } G/A - Sz(C_{2n-1}) &= \sum_{e \in E(C_{2n-1})} \frac{2\sqrt{(n-1)(n-1)}}{(n-1) + (n-1)} \\ &= |E(C_{2n-1})| \\ &= 2n - 1. \text{ Hence follows the result.} \end{aligned}$$

Theorem 2.5: For the path P_n ($n \geq 2$), $G/A - Sz(P_n) = \frac{2}{n} \sum_{i=1}^{n-1} \sqrt{i(n-i)}$.

Proof: Let $V(P_n) = \{v_1, v_2, \dots, v_n\}$. Any edge of P_n is of the form $e_i = v_i v_{i+1}$ for $i = 1 \dots (n-1)$. For any $e_i \in E(P_n)$, by Th.2.2 in [4], $n_1(e_i) = i$ and $n_2(e_i) = (n-i)$.

$$\text{So, } G/A - Sz(P_n) = \sum_{i=1}^{n-1} 2 \frac{\sqrt{i(n-i)}}{(i+n-i)} = \frac{2}{n} \sum_{i=1}^{n-1} \sqrt{i(n-i)}.$$

Corollary 2.6:

$$\text{a) } G/A - Sz(P_{2m}) = \begin{cases} 1 & \text{if } m = 1 \\ \frac{4}{2m} \left(\sum_{i=1}^{m-1} \sqrt{i(2m-i)} + \frac{m}{2} \right) & \text{for } m \geq 2. \end{cases}$$

Observe that, with the convention $\sum_{i=r}^s \dots = 0$ if $s < r$, we get the index of P_2 from the later formula by taking $m = 1$).

$$\text{b) } G/A - Sz(P_{2m+1}) = \frac{4}{2m+1} \left\{ \sum_{i=1}^{m-1} \sqrt{i(2m-i)} \right\} \text{ for } m \geq 1.$$

Proof: By taking $n = 2$ in Theorem (2.5), we get that $G/A - Sz(P_2) = \frac{2}{2} \sqrt{(1)(1)} = 1$.

Let $n \geq 4$ and be even. We can write $n = 2m$ ($m \geq 2$).

$$\begin{aligned} \text{So, } G/A - Sz(P_{2m}) &= \frac{2}{2m} \left(\sum_{i=1}^{2m-1} \sqrt{i(2m-i)} \right) \\ &= \frac{2}{2m} \left(\sum_{i=1}^{m-1} \sqrt{i(2m-i)} + \sqrt{m(2m-m)} + \sum_{i=m+1}^{2m-1} i(2m-i) \right) \end{aligned} \tag{2.6.1}$$

Replacing i by $(2m - i)$ in the third sum of (2.6.1), we observe that

$$\sum_{i=m+1}^{2m-1} i(2m-i) = \sum_{i^1=1}^{m-1} (2m-i^1)(i^1) = \sum_{i=1}^{m-1} \sqrt{i(2m-i)}.$$

Hence, from (2.6.1) we have

$$\begin{aligned} G/A - Sz(P_{2m}) &= \frac{2}{2m} \left[2 \sum_{i=1}^{m-1} \sqrt{i(2m-i)} + m \right] \\ &= \frac{4}{2m} \left[\sum_{i=1}^{m-1} \sqrt{i(2m-i)} + \frac{m}{2} \right]. \end{aligned}$$

This proves (a).

Let $n = 2m + 1$ ($m \geq 1$)

$$\begin{aligned} \text{Now } G/A - Sz(P_{2m+1}) &= \frac{2}{2m+1} \left[\sum_{i=1}^{2m} \sqrt{i(2m+1-i)} \right] \\ &= \frac{2}{2m+1} \left[\sum_{i=1}^m \sqrt{i(2m+1-i)} + \sum_{i=m+1}^{2m} \sqrt{i(2m+1-i)} \right] \end{aligned}$$

Replacing ‘ i ’ by $(2m+1-i)$ in the second sum, as in the previous case, we observe that this sum is same as the first one.

$$\text{So, } G/A - Sz(P_{2m+1}) = \frac{4}{2m+1} \left[\sum_{i=1}^m \sqrt{i(2m+1-i)} \right].$$

This proves (b) and thus the proof of the theorem is complete.

Theorem 2.7: For the wheel

$$K_1 \vee C_n (n \geq 3), G/A - Sz(K_1 \vee C_n) = n \left(1 + \frac{2\sqrt{n-2}}{n-1} \right).$$

Proof: Let $V(K_1 \vee C_n) = \{ u_0, v_1, v_2, \dots, v_n \}$ where u_0 is the centre (hub) of the wheel.

Now, $E(K_1 \vee C_n) = \{ u_0v_i : i = 1, 2, \dots, n \} \cup \{ v_i v_{i+1} : i = 1, 2, \dots, n \}$ (with the convention $v_{n+1} = v_1$).

Denote $e_i = u_0v_i$ and $f_i = v_i v_{i+1}$ ($i = 1, 2, \dots, n$). Now, from Th. 2.7 in [4], for any $e \in E(K_1 \vee C_n)$, $n_1(e) = n - 2$, $n_2(e) = 1$ and observe that the f_i 's constitute C_n .

$$\begin{aligned} \text{So, } G/A - Sz(K_1 \vee C_n) &= \sum_{i=1}^n \frac{2\sqrt{n_1(e_i)n_2(e_i)}}{n_1(e_i) + n_2(e_i)} + G/A - Sz(C_n) \\ &= 2 \sum_{i=1}^n \frac{\sqrt{(n-2)(1)}}{(n-2) + 1} + n \text{ (by virtue of Th.(2.4))} \\ &= \frac{2n}{n-1} \sqrt{(n-2)} + (n) \\ &= n \left(1 + \frac{2\sqrt{n-2}}{n-1} \right). \end{aligned}$$

3. MODIFIED G/A – SZEGED INDEX OF STANDARD GRAPHS

In the calculations of G/A – Szeged indices of K_n ($n \geq 2$), C_{2n-1} ($n \geq 2$) and $K_1 \vee C_n$ ($n \geq 3$) the contribution of all the vertices of the corresponding graphs are not there. To avoid this, we propose the following modified index that involves all the vertices.

Definition 3.1: Let G be a graph and $e = uv \in E(G)$.

Denote $N_1^*(e/G) = \{ w \in V(G) : d(w, u) \leq d(w, v) \}$,

$N_2^*(e/G) = \{ w \in V(G) : d(w, v) < d(w, u) \}$

and

$n_1^*(e/G) = |N_1^*(e/G)|$ & $n_2^*(e/G) = |N_2^*(e/G)|$.

The refined G/A – Szeged Index of G , denoted by $G/A - Sz^*(G)$ is defined as,

$$\sum_{e \in E(G)} \left\{ 2 \frac{\sqrt{n_1^*(e/G).n_2^*(e/G)}}{n_1^*(e/G) + n_2^*(e/G)} \right\}$$

(Another way of defining this modified index is to keep $<$ as it is in $N_1^*(e/G)$ and changing $<$ into \leq in $N_2^*(e/G)$).

Observation 3.2: For the graphs, P_n ($n \geq 2$), $K_{m,n}$ ($m, n \geq 1$), C_{2n} ($n \geq 2$), we observe that this modified index is same as the previous one, since there are no leftout vertices.

Theorem 3.3: For $n \geq 2$, $G/A - Sz^*(K_n) = (n-1)^{3/2}$.

Proof: For any $e \in E(K_n)$, by Th. 3.3 in [4], $n_1^*(e) = n-1$ and $n_2^*(e) = 1$.

$$\begin{aligned} \text{So, } G/A - Sz(K_1 \vee C_n) &= \sum_{e \in E(K_n)} \frac{2\sqrt{(n-1)(1)}}{n-1+1} \\ &= \frac{2}{n} \sqrt{n-1} \left(\frac{n(n-1)}{2} \right) \\ &= (n-1)^{3/2}. \end{aligned}$$

Theorem 3.4: For $n \geq 2$, $G/A - Sz^*(C_{2n-1}) = 2\sqrt{n(n-1)} (\leq 2n-1)$

Proof: For any $e \in E(C_{2n-1})$, by Th. (3.4) in [4], $n_1^*(e_i) = n$ and $n_2^*(e_i) = n-1$.

$$\begin{aligned} \text{So, } G/A - Sz^*(C_{2n-1}) &= \sum_{e \in E(C_{2n-1})} \frac{2\sqrt{n(n-1)}}{(n+n-1)} \\ &= \frac{2}{2n-1} \sqrt{n(n-1)} |E(C_{2n-1})| \\ &= \frac{2}{2n-1} \sqrt{n(n-1)}(2n-1) \\ &= 2\sqrt{n(n-1)} (\leq 2n-1) \text{ (since G.M. } \leq \text{A.M.)} \end{aligned}$$

Observation 3.5: In the other way of defining the modified index, we get the same indices for K_n and C_{2n-1} since $n_1^*(e)$ and $n_2^*(e)$ are interchanged in the corresponding calculations.

Theorem 3.6: For the wheel $K_1 \vee C_n$ ($n \geq 3$),

$$G/A - Sz^*(K_1 \vee C_n) = \begin{cases} \frac{2n}{n+1} \left[\sqrt{n} + \sqrt{\frac{n}{2} \left(\frac{n}{2} + 1\right)} \right] & \text{if } n \text{ is even,} \\ \frac{n}{n+1} \left[2\sqrt{n} + \sqrt{n^2 + 2n - 3} \right] & \text{if } n \text{ is odd.} \end{cases}$$

Proof: With the same notation of Th 2.7, $n_1^*(e_i) = n-2+2 = n$ and $n_2^*(e_i) = 1$.

So,

$$\sum_{i=1}^n \frac{2\sqrt{n_1^*(e_i)n_2^*(e_i)}}{n_1^*(e_i) + n_2^*(e_i)} = \frac{2n}{n+1} \sqrt{n} \tag{3.6.1}$$

Case (i): Suppose n is even.

By Th. 3.6.1 in [4], we have

$$n_1^*(f_i) = n/2 + 1 \text{ and } n_2^*(f_i) = n/2$$

So

$$\sum_{i=1}^n \frac{2\sqrt{n_1^*(f_i)n_2^*(f_i)}}{n_1^*(f_i) + n_2^*(f_i)} = \frac{2}{n+1} n \sqrt{\frac{n}{2} \left(\frac{n}{2} + 1\right)} \tag{3.6.2}$$

By (3.6.1) and (3.6.2)

$$G/A - Sz^*(K_1 \vee C_n) = \frac{2n}{n+1} \left[\sqrt{n} + \sqrt{\frac{n}{2} \left(\frac{n}{2} + 1\right)} \right].$$

Case (ii): Suppose n is odd.

By Th.3.6.2 in [4],

$$n_1^*(f_i) = \frac{n-1}{2} + 2 = \frac{n+3}{2} \text{ and } n_2^*(f_i) = \frac{n-1}{2}.$$

$$\begin{aligned} \text{So, } \sum_{i=1}^n \frac{2\sqrt{n_1^*(f_i)n_2^*(f_i)}}{n_1^*(f_i) + n_2^*(f_i)} &= \frac{2n}{n+1} \sqrt{\left(\frac{n+3}{2}\right)\left(\frac{n-1}{2}\right)} \\ &= \frac{n}{n+1} \sqrt{n^2 + 2n - 3} \end{aligned} \tag{3.6.3}$$

By (3.6.1) and (3.6.3)

$$G/A - Sz^*(K_1 \vee C_n) = \frac{n}{n+1} \left[2\sqrt{n} + \sqrt{n^2 + 2n - 3} \right]$$

This completes the proof of the theorem.

Observation 3.7: In the otherway of defining the modified Index, we get that $(n_1^*(e_i) = (n - 2)$ and $(n_2^*(e_i) = 3$ and the other relations remain the same. So,

$$\sum_{i=1}^n \frac{2\sqrt{n_1^*(e_i)n_2^*(e_i)}}{n_1^*(e_i) + n_2^*(e_i)} = \frac{2n}{n+1} \left[\sqrt{3(n-2)} \right]$$

$$\text{Hence, } G/A - Sz^*(K_1 \vee C_n) = \begin{cases} \frac{2n}{n+1} \left[\sqrt{3(n-2)} + \sqrt{\frac{n}{2} \left(\frac{n}{2} + 1 \right)} \right] & \text{if } n \text{ is even,} \\ \frac{n}{n+1} \left[2\sqrt{3(n-2)} + \sqrt{n^2 + 2n - 3} \right] & \text{if } n \text{ is odd.} \end{cases}$$

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